Globally singularity free semi-classical wave functions in closed form

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Abstract

We use a factorisation technique and representations of canonical transformations to construct globally valid closed form expressions without singularities of semi-classical wave functions for arbitrary smooth local potentials over a one-dimensional position space.

1 Introduction

In semi-classical treatments we construct approximate solutions of a quantum mechanical problem from the knowledge of the solutions of the corresponding classical problem. The usual WKB procedure yields excellent results sufficiently far away from turning points. Yet at turning points this approximation leads to singularities. This occurs for all energies below the maximal value of the potential. Furthermore degenerate situations occur at maxima of this potential. Some kind of regularisation (uniformisation) is used near such points. The most common ad hoc solution uses Airy functions near turning points and Pearcy functions near maxima [1].

The purpose of this paper is to present a semi-classical global approximation without singularities. To achieve this we take advantage of the following facts:

First, the solution of a problem linear in momentum such as $p + V(q) - E = 0$ is trivial under canonical quantisation. Second, the usual Hamiltonian $H = p^2/2 + V(q)$ can be factorised into two factors of the first type. Third one of these factors can be converted to a simple momentum by a canonical transformation. For quantum mechanics we need Fourier and gauge transformations [2]. Their composition introduces errors of order $\hbar^2$ thus leading to an integral representation of an approximate solution. A judicious selection of the integration path depending on the coordinate yields converging integrals everywhere, thus guaranteeing a uniform approximation.

We shall show, that the saddle point approximation of the integral again yields the WKB solution, and indicate how the path of integration has to be laid to avoid singularities at turning points and extremal points of the potential. We will restrict our discussion to the one dimensional case and a Hamiltonian with local potential, where the action for a given energy E is defined as

$$S(q) = \int^q ds[2(E - V(s))]^{1/2} \tag{1}$$

2 The factorisation

We start by introducing the function $\Omega(q,p,E) = H(q,p) - E$. Then the wave function is an eigenfunction with eigenvalue 0 of the operator version of Ω under the usual canonical quantisation. If Ω were linear in p, we could bring it into the form

$$\Omega = p - g(q,E) \tag{2}$$

where g is the derivative of the action function (which would have only one branch in this case) and the exact wave function would have the simple form

$$\psi(q) = c\ \exp[iS(q)/\hbar] \tag{3}$$

For Hamiltonian functions of the standard form Ω is a polynomial of second degree in p and after multiplication by 2 we can decompose it into the linear factors

$$\Omega = [p - g(q,E)] * [p + g(q,E)] \tag{4}$$

where the two functions g are the derivatives of the two branches of the action function which differ only in their sign. It is again trivial to construct eigenfunctions with eigenvalue 0 for each factor. But this does not solve the entire problem because of the ordering problem of quantum mechanics. In order to obtain an hermitian operator we must write the factors in some symmetrical order, and there are infinitely many ways to do so. Fortunately they only differ in $\hbar^2$ and higher orders in $\hbar$. Since we want to construct semi-classical solutions all these possibilities are equally correct for our purpose and we can select the one which is most convenient. We choose

$$\Omega = [p - g(q,E)]^{1/2} * [p + g(q,E)] * [p - g(q,E)]^{1/2} \tag{5}$$

Next we remember, that for canonical transformations which are represented by gauge transformations, this representation is quantum mechanically precise [2]. At this stage it helps to apply the following canonical transformation

$$p \to p + g(q,E),\ q \to q \tag{6}$$

to bring Ω into the form

$$\Omega = p^{1/2}[p + 2\,g(q,E)]p^{1/2} \tag{7}$$

Now assume that $\tilde{\chi}(p)$ is the Fourier transform of the wave function $\chi(q)$, which is eigenfunction with eigenvalue 0 of the operator version of $[p + 2\,g(q,E)]$. Then $\tilde{\phi}(p) = p^{-1/2}\tilde{\chi}(p)$ is eigenfunction with eigenvalue 0 of the operator version of Ω of Eq. 7 in momentum representation.

3 Construction of the wave function

To obtain an expression for the final wave function $\psi(q)$ we have to assemble all steps in reverse order. First it is obvious that the function $\chi(q)$ has the form

$$\chi(q) = c\exp[i(2\,S(q,E)/\hbar] \tag{8}$$

such that its Fourier transform

$$\tilde{\chi}(p) = c\int dr \exp[i(rp + 2\,S(r,E)/\hbar] \tag{9}$$

yields $\tilde{\chi}(p)$ as used above, Here, and in what follows, we put all uninteresting factors into the normalisation constant c. According to Eq. 8 we obtain $\tilde{\phi}(p)$ and next $\phi(q)$ by an inverse Fourier transform as

$$\phi(q) = c\int dp \int dr p^{-1/2} \exp[i(-qp + rp + 2\,S(r,E))/\hbar] \tag{10}$$

The p integral can be done in closed form giving

$$\phi(q) = c \int dr \mid q - r \mid^{-1/2} \exp[2i\, S(r,E)/\hbar] \tag{11}$$

Now we make a substitution of the integration variable introducing s as new integration variable according to $r = q - s^2$ arriving at

$$\phi(q) = c \int ds \exp[2i\, S(q - s^2, E)/\hbar] \tag{12}$$

Finally to arrive at $\psi(q)$ we must undo the canonical transformation Eq. 6. This is done by multiplying the wave function by the gauge factor $\exp[-i\, S(q,E)/\hbar]$ and we obtain

$$\psi(q) = c \exp[-i\, S(q,E)/\hbar] \int ds \exp[2i\, S_2(q - s^2, E)/\hbar] \tag{13}$$

This is the formal global solution we wished to obtain, once we determine the path of integration. Yet for formal manipulations the fact that we have this closed form may be quite important. For example we can readily see that we retrieve the WKB approximation by a power expansion, as long as we are far away from any turning point. Then we formally expand $S(q - s^2, E)$ in a power series in s^2 and only keep the first two terms giving $S(q,E) - s^2 \partial S(q,E)/\partial q$. Plugging in into Eq. 21 gives

$$\begin{aligned} \psi(q) &= \exp[-iS(q,E)/\hbar] \int ds \exp[2is^2 \partial S(q,E)/\partial q/\hbar] \\ &= c(\partial S(q,E)/\partial q)^{-1/2} \exp[-iS(q,E)/\hbar] \end{aligned} \tag{14}$$

which is the usual WKB solution. To arrive at this result we have taken the stationary phase contribution of the point $s = 0$ to the s integral. The exponent can have further stationary points at values s_c of s such that $q - s_c^2$ is a turning point. However, in general, S varies as $(s - s_c)^{3/2}$ in the vicinity of such argument values; therefore its second derivative goes as $(s - s_c)^{-1/2}$. Accordingly, the contribution of such points to the saddle point evaluation of the integral has weight zero. Therefore the point $s = 0$ is the only point giving contributions in saddle point evaluation of the integral.

4 The integration path

We have started from a second order differential equation. Therefore we must be able to obtain two linearly independent solutions. One way is to reverse the sign of S, the other is by appropriate choices of the integration path for the variable s in the complex plane. The integrand is the exponential of some function $f(s)$, the square bracket in Eq. 20. Along some sectors for the angle α of the complex variable s the function $f(s)$ acquires large negative real parts and the integrand decays exponentially. Let us call these intervals I_j. For the sectors in between the integrand explodes exponentially. An appropriate choice for the integration path is to come in from infinity in one angle sector I_{in}, to pass near the origin and to return to infinity in a different sector I_{out}. Some combinations of the two intervals will produce the same solution, and some the solution identically zero. But there should be two different choices leading to two different solutions. In general the function $f(s)$ can have isolated singularities, whose position depends on q and E. Then we may eventually deform the integration path into one, encircling some of these singularities.

By a good choice of the integration path we can also be sure that the solution does not have singularities. To understand this, let us fix a value of E and consider q in a small neighbourhood of an arbitrary fixed point q_0. Assume for the moment that the potential $V(q)$ is an analytic function. Then the integrand may have some singularities in isolated points in s, but outside of them it is analytic. We call the singular points s_j. As we vary q the singular points in s will also move in

general but remain in small neighbourhoods of $s_j(q_0)$. When we choose the integration path such that it avoids all these little neighbourhoods, then we obtain a function $\psi(q)$ which is analytic in the neighbourhood of the point q_0. When we vary q over large ranges, then we have eventually to shift the integration path accordingly to avoid singularities.

The two most important situations where we need the explicit path of the integral are near the maximum of potentials and near turning points. It can be shown that in the first case, if we use the quadratic approximation for the extremum we retrieve the exact solution, *i.e.* the Pearcy function. In the second case it does not seem easy to find a path that yields the exact solution, but by choosing a path that fulfills the above conditions, we obtain a solution that has no singularities and numerical inspection shows it to be quite close to the Airy function.

5 Conclusions

We have obtained an integral representation for a semi-classical approximation, of the wave-function of a standard Hamiltonian with local potential. The method involves a factorisation, which causes errors in higher orders of $\hbar$, which is acceptable for a semi-classical approximation. As we may expect the usual WKB method results from a saddle-point approximation of this integral. Judicious choices of the path of the integral in the complex plane lead to approximate solutions which have no singularities and thus converge everywhere adequately. The method may be readily generalized to Hamiltonians which are of higher order in the momenta. In particular examples it might be useful to modify the method slightly by multiplying and dividing by additional factors. This can in many cases provide the exact solution for all values of the energy. In a future publication we will present such examples in detail.

The advantages of this method consist in the fact that the points where WKB breaks down are not treated piecemeal, but are covered by the same integral representation. Whenever we wish to make an analytic statement about semi-classics this can be a great advantage.

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References

[1] J. Connor, Mol. Phys. 26, 1217 (1973); J. Connor and D. Farrelly, J. Chem. Phys. 75, 2831 (1981)

[2] C. Jung and H. Krüger, J. Phys. A **15**, 3509 (1982); **16**, 1379 (1983); **17**, 1033 (1984); F. Leyvraz T.H. and Seligman J. Math. Phys. **30**, 2512 (1989)